NONLINEAR OSCILLATIONS OF TWO COUPLED COMPLEMENTARY DNA BASES

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Nonlinear large amplitude oscillations of DNA base pairs, in which adenine forms two hydrogen bonds with thymine, and guanine forms three hydrogen bonds with cytosine, are of special interest, because they made substantial contribution to the process of opening DNA base pairs and that, in turn, is considered as one of important elements of the process of the DNA-protein recognition.

In order to study the oscillations we develop and modify the recently proposed approach, and we apply it to study nonlinear oscillations of single DNA bases: Adenine (A), Thymine (T), Guanine (G) and Cytosine (C) (see [1]).

We show that the dynamical equations that govern the DNA base pair oscillations have the form

$$I_1 \frac{d^2\varphi_1}{dt^2} + \frac{1}{2} K_{12}[A_1 \sin\varphi_1 - B\sin(\varphi_1 + \varphi_2)] = -\beta \frac{d\varphi_1}{dt} + F,$$

$$I_1 \frac{d^2\varphi_2}{dt^2} + \frac{1}{2} K_{12}[A_2 \sin\varphi_2 - B\sin(\varphi_1 + \varphi_2)] = -\beta \frac{d\varphi_2}{dt} + F,$$

where φ_1 and φ_2 are the angles of inclination of the 1-st and 2-nd complementary bases from their equilibrium positions; I_1 and I_2 are the moments of inertia of the bases; K_{12} is the parameter characterizing interactions between the bases; $A_1 = 2\, r_1(r_1 + r_2 + a)$; $A_2 = 2\, r_2(r_1 + r_2 + a)$; $B = 2\, r_1 r_2$; r_1 and r_2 are the distances between the centers of mass of the bases and the sugar-phosphate chains; a is the distance between masses of pendulums in the equilibrium state ($\varphi_1 = \varphi_2 = 0$); β is the coefficient of dissipation, and F is an external generalized force.

We obtain the solutions of the equations and the trajectories of the investigated system in the phase space for both cases: AT and GC base pairs.

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References

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